Amendments to the Claims

This listing of claims will replace all prior versions, and listings, of the claims in the application:

Listing of Claims

1. (withdrawn) A method of analysing chemical data including a step of cluster analysis, the cluster analysis using a distance metric of the form:

$$D_{xy} = \frac{\sum_i \left(\left(\frac{x_i - c_i}{s_i} \right) - \left(\frac{y_i - c_i}{s_i} \right) \right)^2}{\sqrt{\left(\sum_i \left(\frac{x_i - c_i}{s_i} \right)^2 \right) \times \left(\sum_i \left(\frac{y_i - c_i}{s_i} \right)^2 \right)}}.$$

2. (withdrawn) A method according to claim 1 that includes a step of performing principal component analysis on the data prior to the clustering step.

3. (withdrawn) A method according to claim 1 that further includes a step of normalising the data prior to the clustering step.

4. (withdrawn) A method according to claim 3 in which the normalising step modifies the data such that it has a mean value of 0 and a standard deviation of 1.

5. (withdrawn) A method according to claim 1 that includes a further step of cluster analysis using a conventional distance metric.

6. (withdrawn) A method according to claim 5 in which the further step of cluster analysis is applied to data that has not previously been assigned to a cluster.

7. (withdrawn) A method according to claim 6 suitable for operation upon a set of data derived from the results of a chemical analysis programme.

8. (withdrawn) A method according to claim 7 in which the analysis programme includes one or both of a quantitative structure-activity relationship (QSAR) analysis and a quantitative structure-property relationship (QSPR) analysis.

9. (currently amended) A method of analysing on a computer 2-dimensional or 3-dimensional chemical data including ~~a step~~ the steps of

cluster analysis on the ~~2-dimensional or 3-dimensional~~ data, the cluster analysis using a distance metric for the distance between point x and point y of the form:

$$D(x,y) = 4\sin^2\left(\frac{\alpha}{2}\right) + \frac{(r_x - r_y)^2}{r_x r_y}$$, where α is the angle between point x and point y and r_x and r_y are, respectively, the distances from the co-ordinate origin to point x and point y; and

outputting the results of the cluster analysis from the computer.

10. (original) A method according to claim 9 that includes a step of performing principal component analysis on the data prior to the clustering step.

11. (original) A method according to claim 9 that further includes a step of normalising the data prior to the clustering step.

12. (original) A method according to claim 11 in which the normalising step modifies the data such that it has a mean value of 0 and a standard deviation of 1.

13. (original) A method according to claim 9 that includes a further step of cluster analysis using a conventional distance metric.

14. (canceled)

15. (original) A method according to claim 9 suitable for operation upon a set of data derived from the results of a chemical analysis programme.

16. (original) A method according to claim 15 in which the analysis programme includes one or both of a quantitative structure-activity relationship (QSAR) analysis and a quantitative structure-property relationship (QSPR) analysis.

17. (withdrawn) A computer program product for performing analysis of chemical data, the program being operative to perform a method including a step of cluster analysis, the cluster analysis using a distance metric of the form:

$$D_{xy} = \frac{\sum_i \left(\left(\frac{x_i - c_i}{s_i} \right) - \left(\frac{y_i - c_i}{s_i} \right) \right)^2}{\sqrt{\left(\sum_i \left(\frac{x_i - c_i}{s_i} \right)^2 \right) \times \left(\sum_i \left(\frac{y_i - c_i}{s_i} \right)^2 \right)}}.$$

18. (withdrawn) A computer program product according to claim 17 that has as an input a set of machine-readable data representative of the results of a chemical analysis programme.

19. (withdrawn) A computer program product according to claim 18 in which the analysis programme includes a quantitative structure-activity relationship (QSAR) analysis and a quantitative structure-property relationship (QSPR) analysis.

20. (currently amended) A computer program product for performing on a computer analysis of 2-dimensional or 3-dimensional chemical data, the program being operative to perform a method including ~~a step~~ the steps of

cluster analysis on the ~~2-dimensional or 3-dimensional~~ data, the cluster analysis using a distance metric for the distance between point x and point y of the form:

$$D(x,y) = 4\sin^2\left(\alpha/2\right) + \frac{(r_x - r_y)^2}{r_x r_y}, \text{ where } \alpha \text{ is the angle between point } x \text{ and point } y$$

and r_x and r_y are, respectively, the distances from the co-ordinate origin to point x and point y; and

outputting the results of the cluster analysis from the computer.

21. (original) A computer program product according to claim 20 that has as an input a set of machine-readable data representative of the results of a chemical analysis programme.

22. (original) A computer program product according to claim 21 in which the analysis programme includes a quantitative structure-activity relationship (QSAR) analysis and a quantitative structure-property relationship (QSPR) analysis.